PRINCÍPIOS DA MECÂNICA QUÂNTICA

ORBITAIS

Modelo de Bohr:

- Átomo de hidrogênio

- Átomos mono-eletrônicos: He^{+}, Li^{2+}

- Estrutura fina espectros: *orbitas elípticas*

Louis de Broglie:

Todos os objetos em movimento apresentam propriedades ondulatórias (1925)

$$mc^2 = h\nu \quad \text{(i)}$$

$$mc^2 = h\frac{c}{\lambda} \quad \text{ou} \quad mc = \frac{h}{\lambda} \quad \text{(ii)}$$

Generalizando a equação ii para uma partícula de velocidade v:

$$mv = \frac{h}{\lambda} \quad \text{(iii)}$$

$$\lambda = \frac{h}{mv} \quad \text{(iv)}$$

Determinação comprimento de onda do Gianluca:

Dados:

Massa= 94kg

Velocidade= 10km/h = 10000 m/3600 s= 2,8m.s^{-1}

Constante de Planck (h)= 6,63x10^{-34} kg.m^2.s^{-1}

$$\lambda = \frac{h}{mv} = \frac{6{,}63\text{x}10^{-34}\ \text{kg.m}^2.\text{s}^{-1}}{94\text{kg}.2{,}8\text{m.s}^{-1}} = 2{,}5\text{x}10^{-36}\,\text{m} = 2{,}5\text{x}10^{-27}\,\text{nm}$$

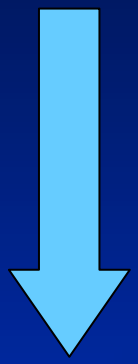
Comprimento de Onda do Elétron:

Massa: $9{,}1\text{x}10^{-31}$ kg

Velocidade: $3\text{x}10^{6}$ m.s^{-1}

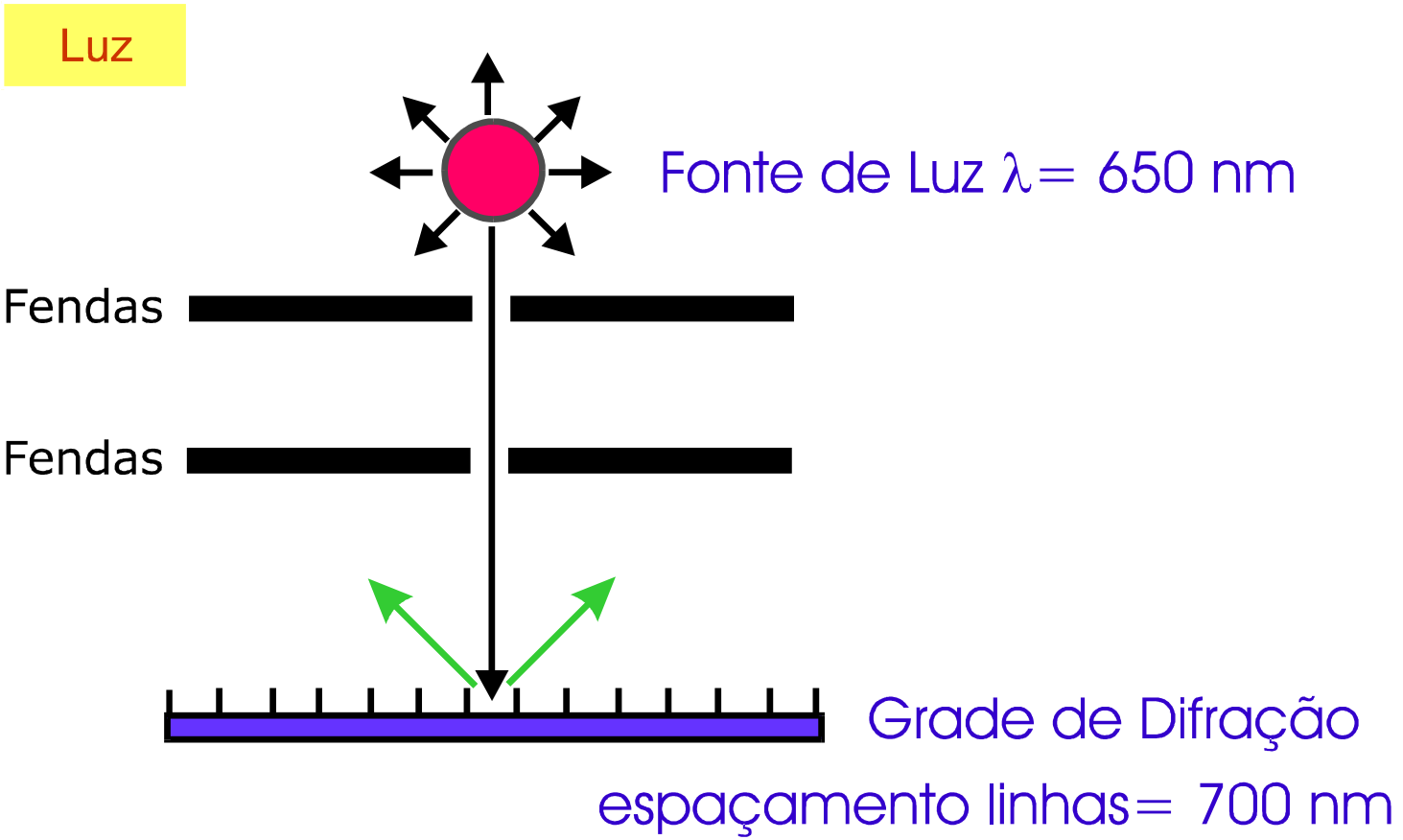
$$\lambda = \frac{h}{mv} = \frac{6{,}63\text{x}10^{-34}\ \text{kg.m}^2\text{.s}^{-1}}{9{,}1\text{x}10^{-31}\,\text{kg}.3{,}0\text{x}10^{6}\,\text{m.s}^{-1}} = 2{,}4\text{x}10^{-11}\,\text{m} = 0{,}24\,\text{nm}$$

DIFRAÇÃO

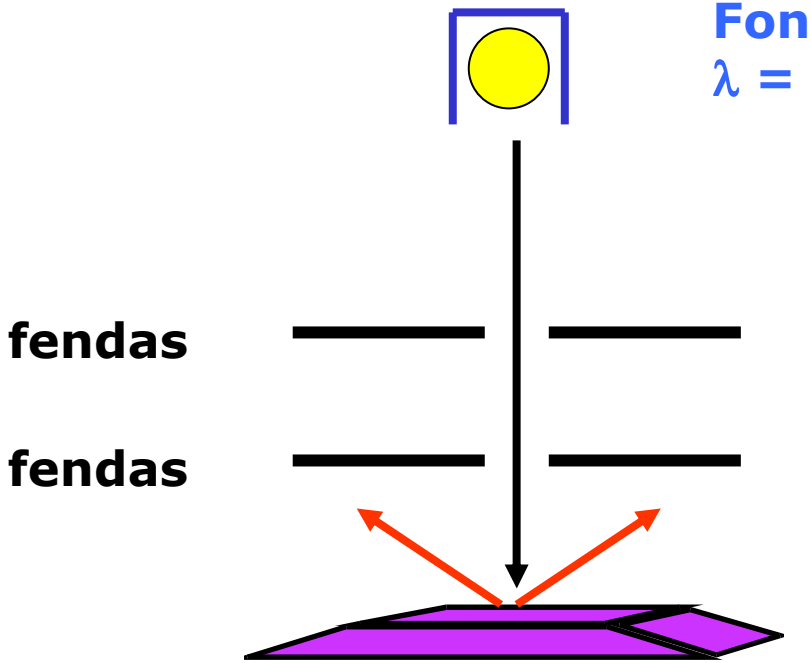


FENÔMENO ONDULATÓRIO

Fenômenos de Difração



1927: Davisson e Germer

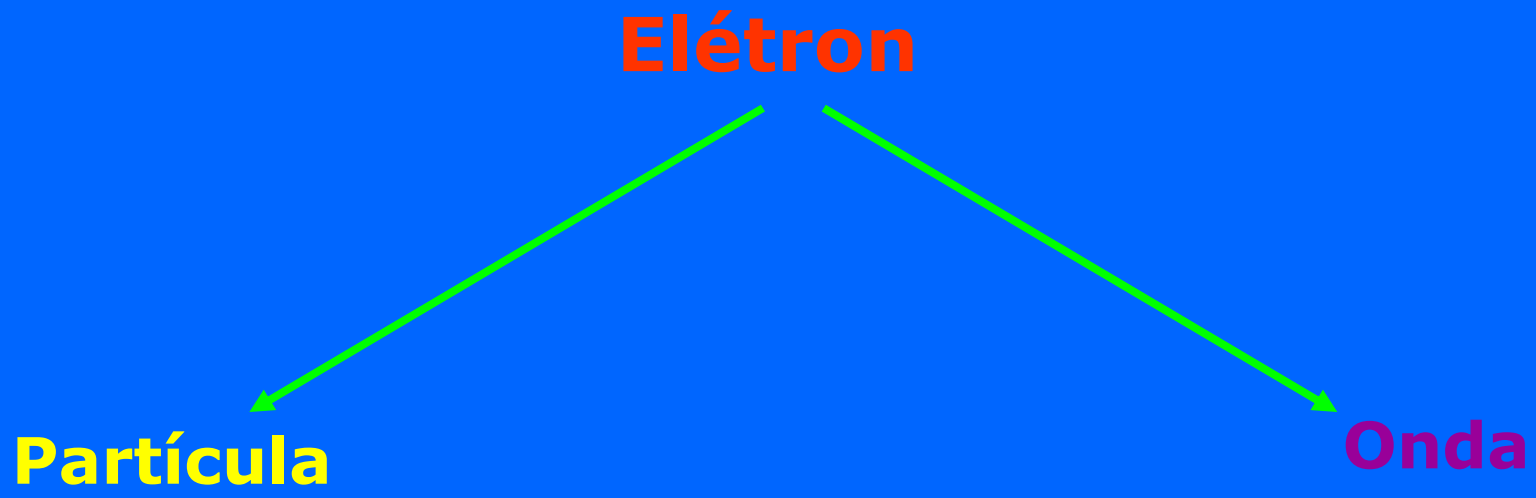


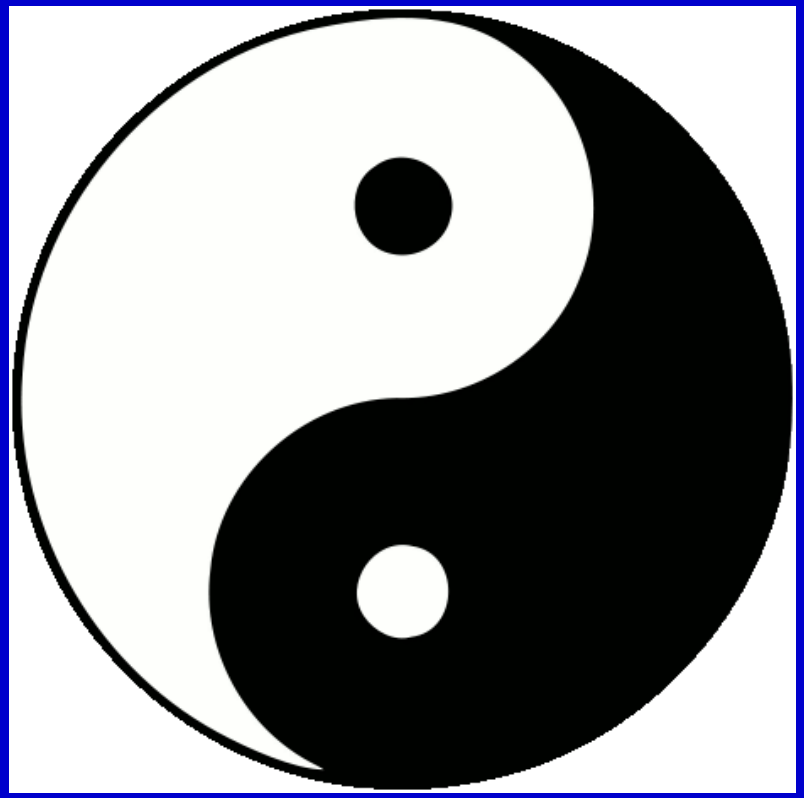
Fonte de elétrons
λ = 0,2 nm

Cristal de níquel:

espaçamento entre os átomos 0,22 nm

Dualidade Partícula - Onda



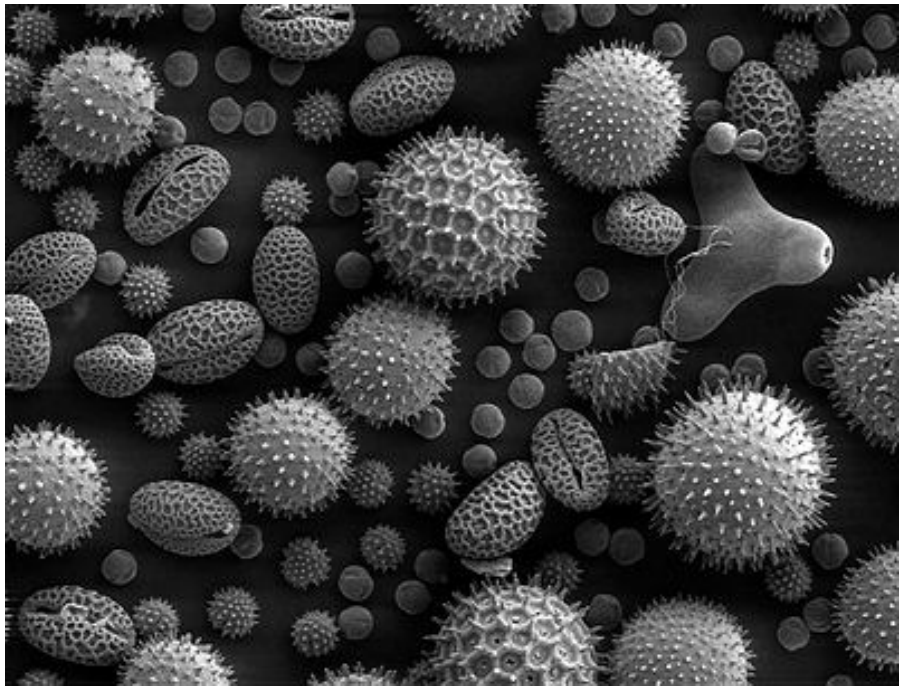


Yin -Yang

Microscopia Eletrônica

"Buque" SiCGa (3D)

Si em matrix polimérica




ANTARCTICA
Head of an Antarctic Mite
Photograph by Gerry Nash

Princípio da Incerteza de Heisenberg

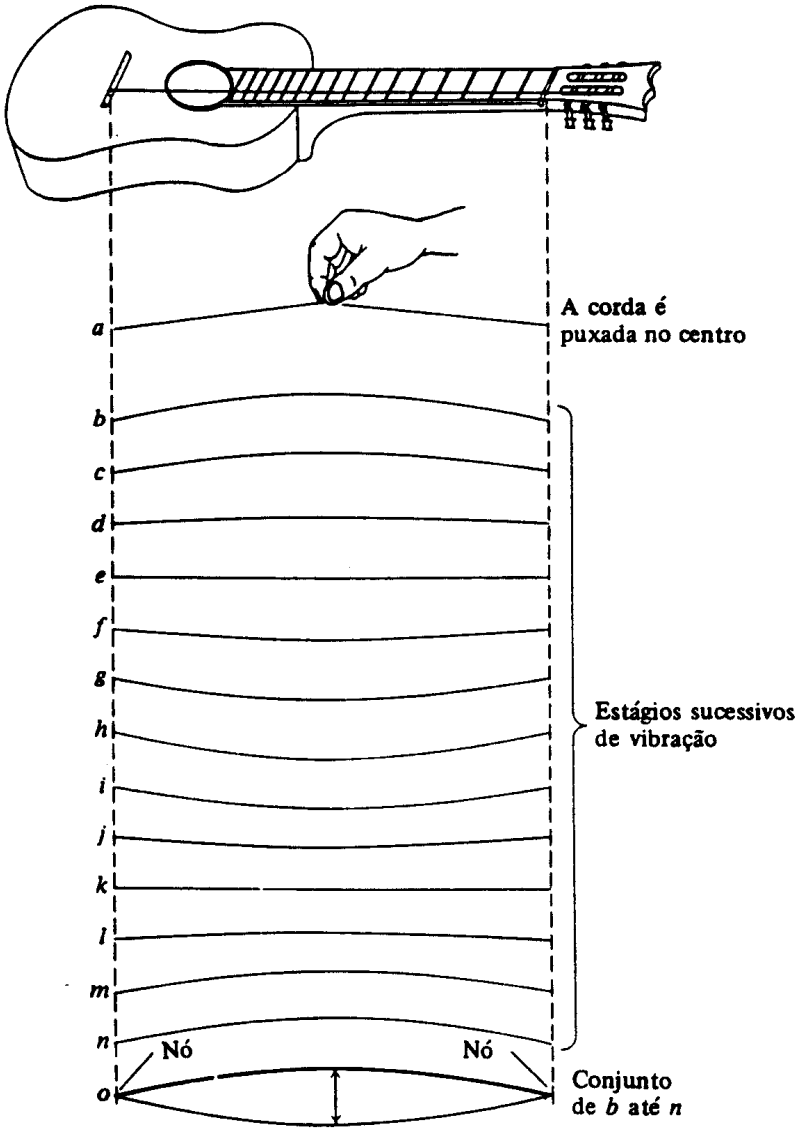
$$\Delta x.\Delta \mathrm{v} \geq \frac{h}{4\pi}$$

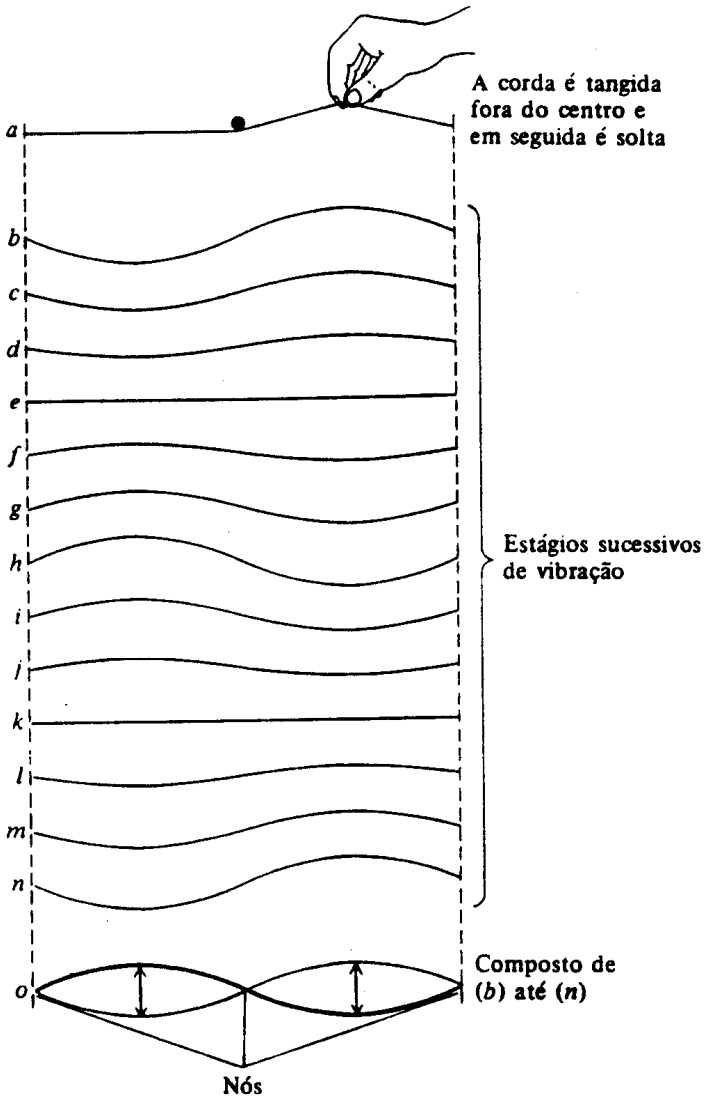
Erwin Schrödinger

Prêmio Nobel em Física 1933

Mecânica Ondulatória

Tratamento do elétron
como onda estacionária


a
b
c
d
e
f
g
h
i
j
k
l
m
n
o
A corda é puxada no centro
Estágios sucessivos de vibração
Nó
Nó
Conjunto de b até n


a
b
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h
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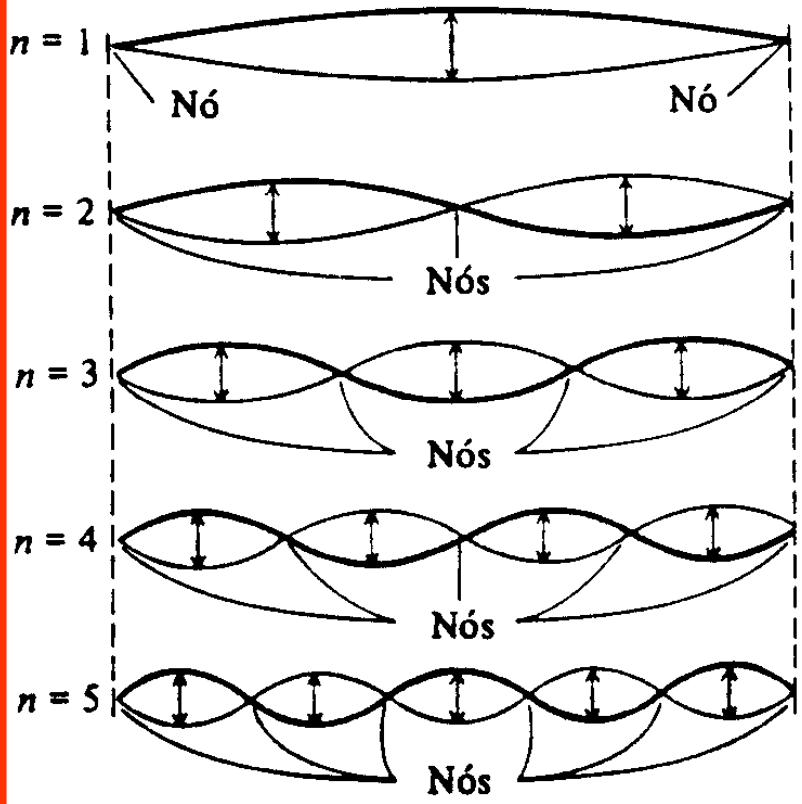
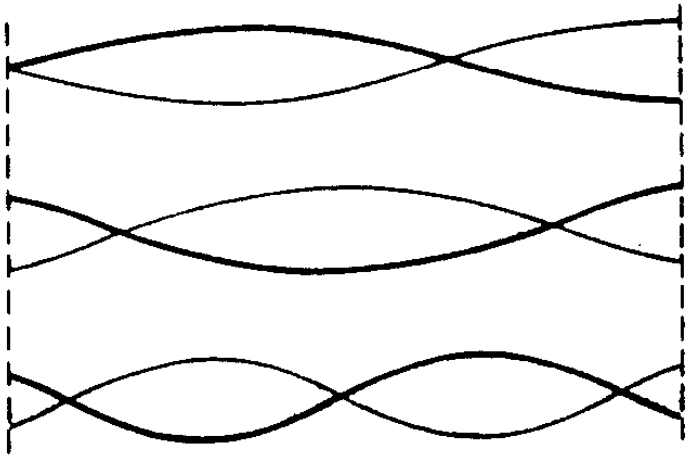
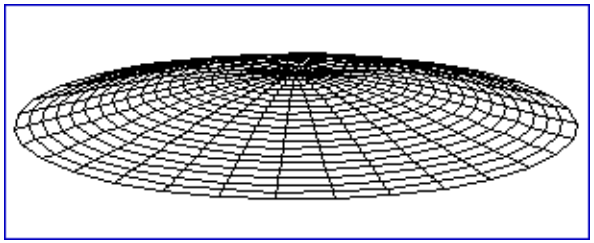
l
m
n
o
A corda é tangida fora do centro e em seguida é solta
Estágios sucessivos de vibração
Composto de (b) até (n)
Nós

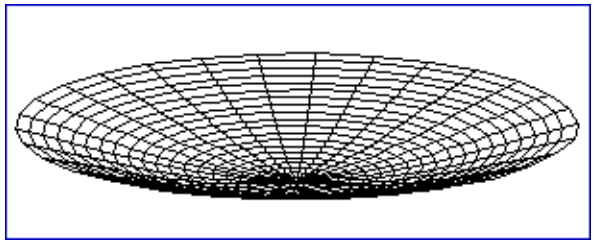
Modos Permitidos de Vibração

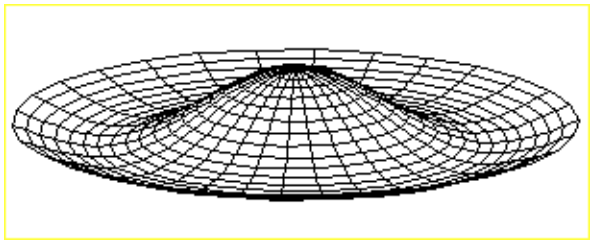
Modos Proibidos de Vibração

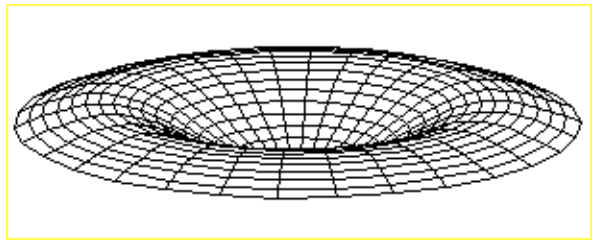


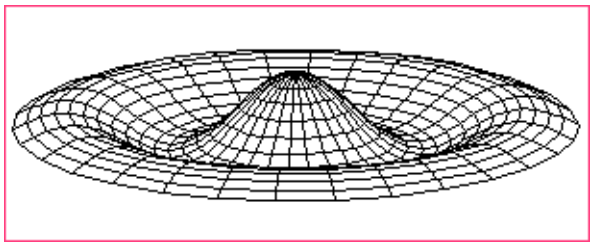


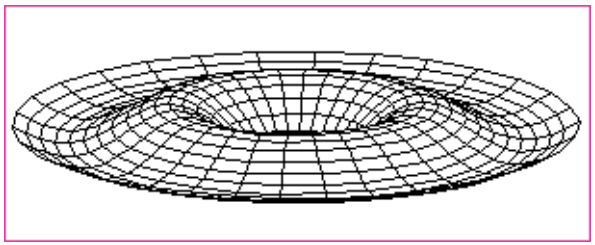


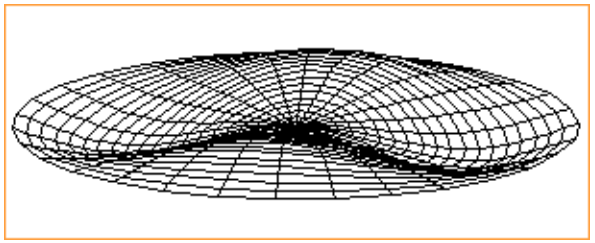


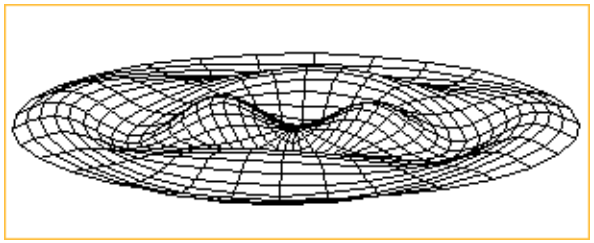


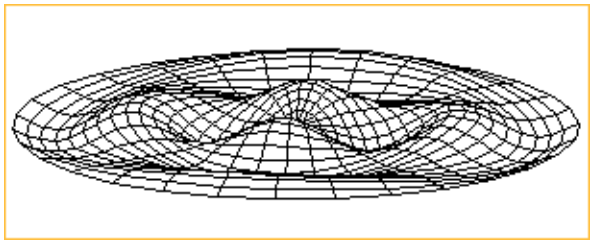




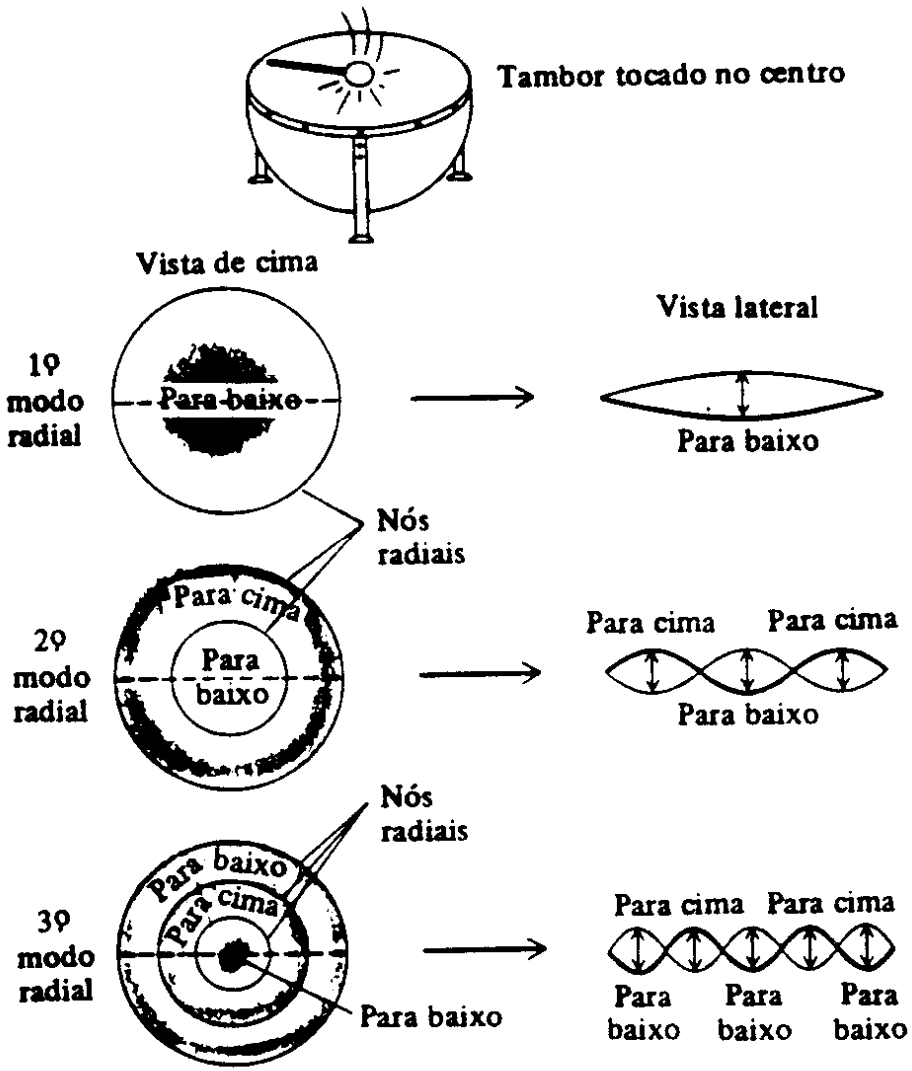


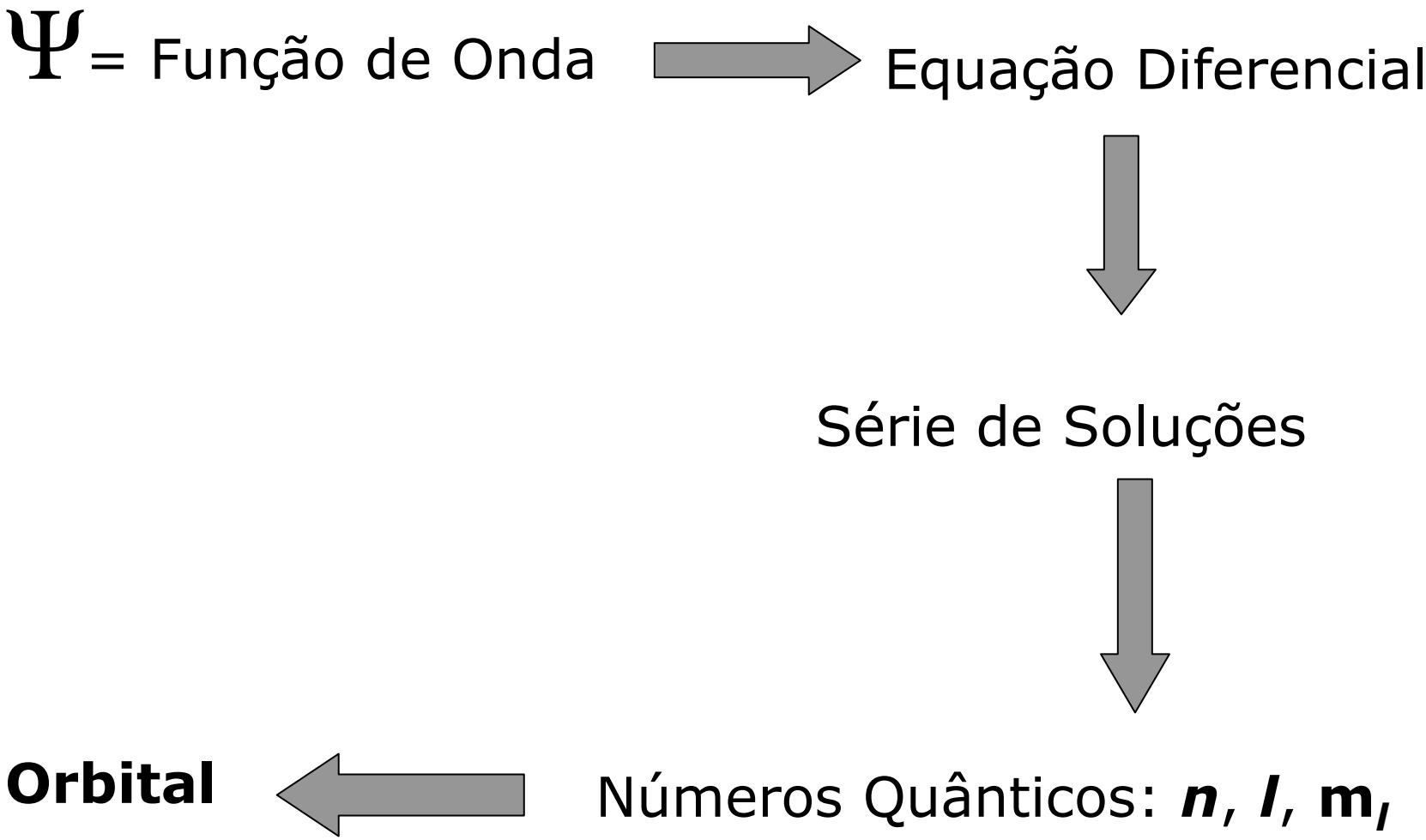






Onda estacionária Bidimensional

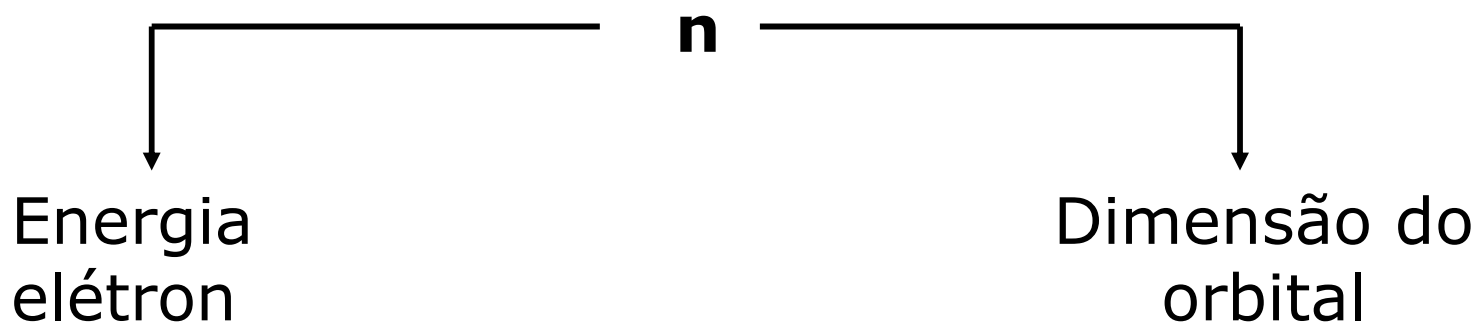



Ψ = Função de Onda
Equação Diferencial
Série de Soluções
Números Quânticos: n, l, m_l
Orbital

Significado dos Números Quânticos

n Número Quântico Principal:
define grupos de orbitais
distintos pelos valores de l e ml

n= 1, 2, 3, 4.....



l número quântico de momento angular (secundário, azimutal)

Define a forma do orbital

Assume valores de 0, 1, 2, 3....n-1

0= s

1= p

2= d

3= f

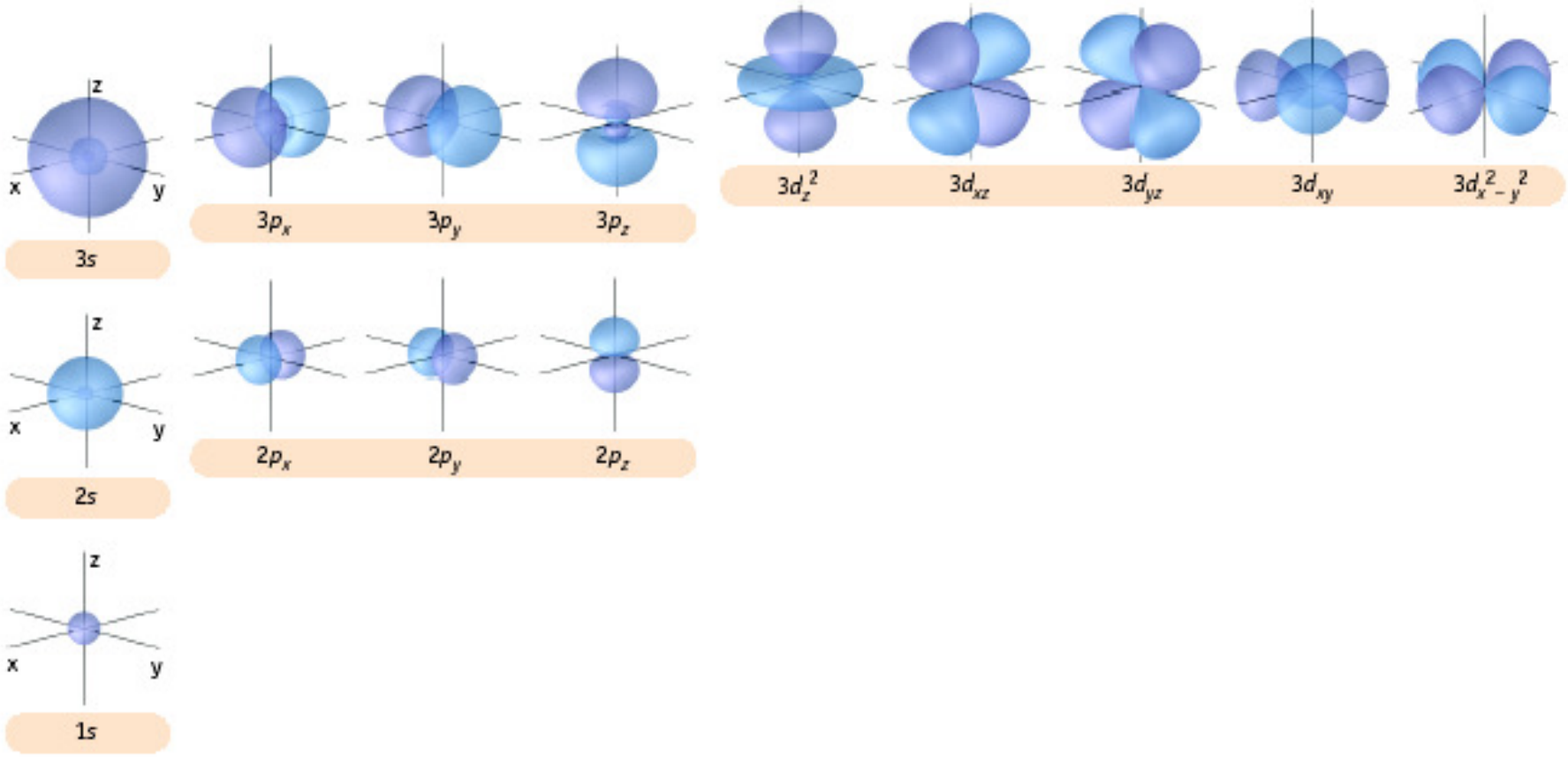
m_l número quântico magnético

Define orientação do orbital

Relacionado ao comportamento do orbital perante um campo magnético externo

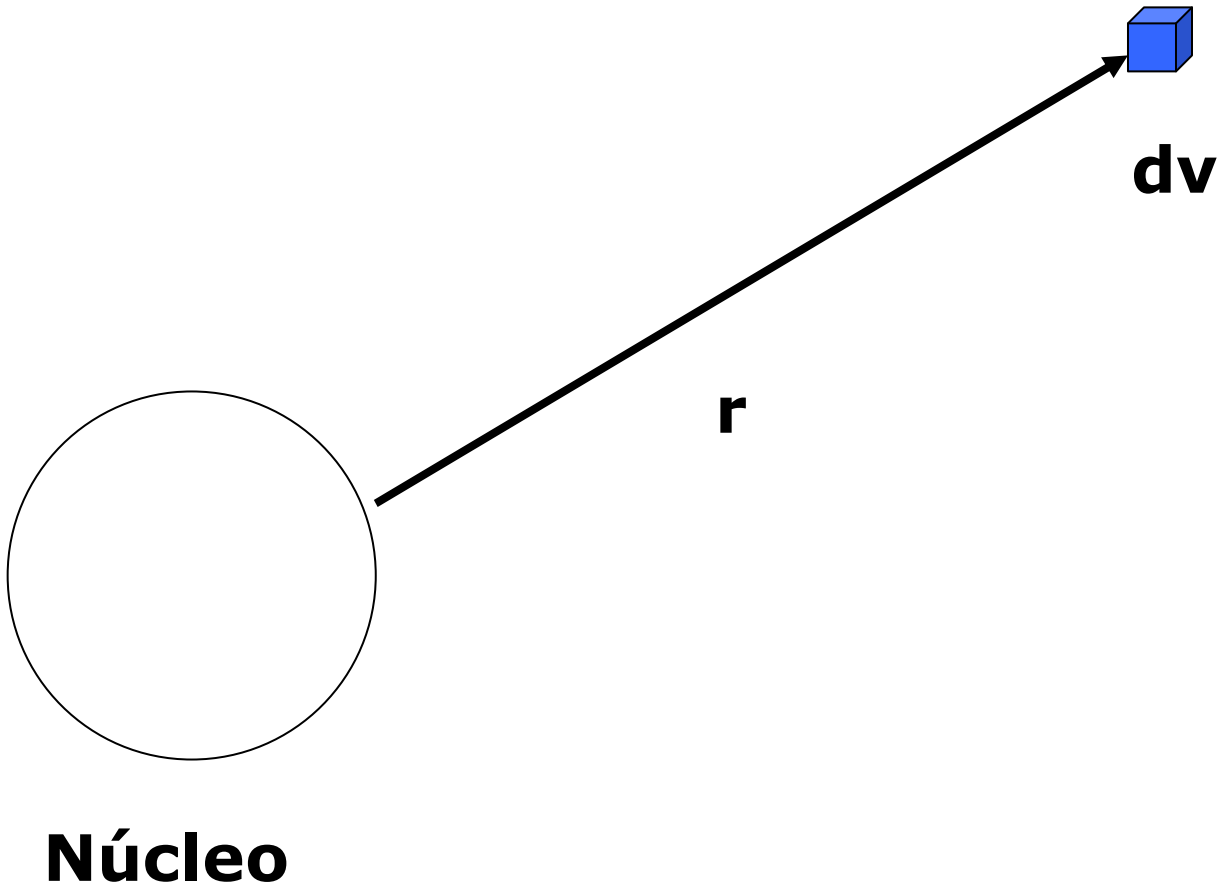
-l, ...-2, -1, 0, 1, 2,.....l

Tipos de Orbitais Atômicos



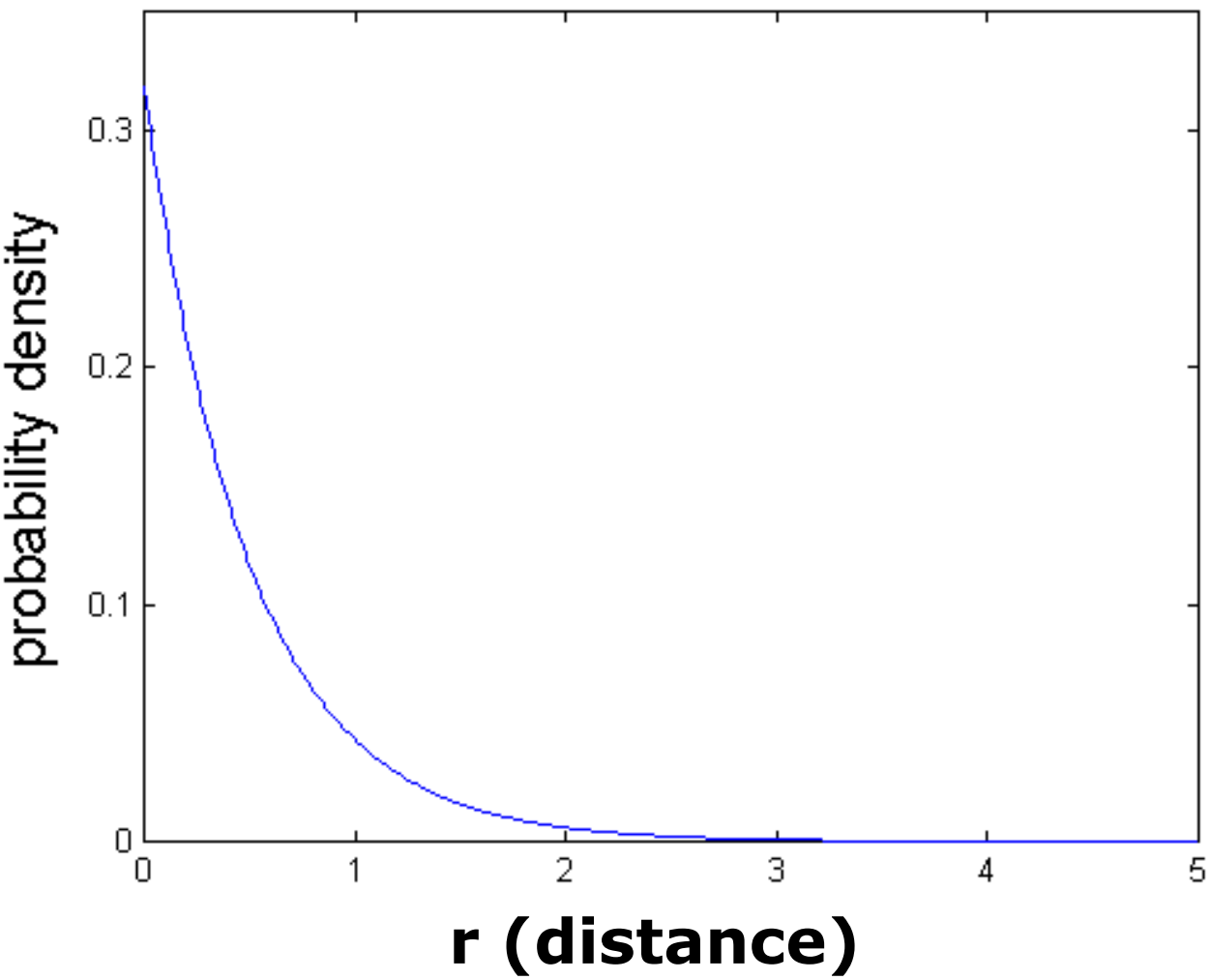
Ψ^2 = Função de Densidade de Probabilidade

Probabilidade de encontrar um elétron em função da distância ao núcleo considerando um volume "pontual" dv

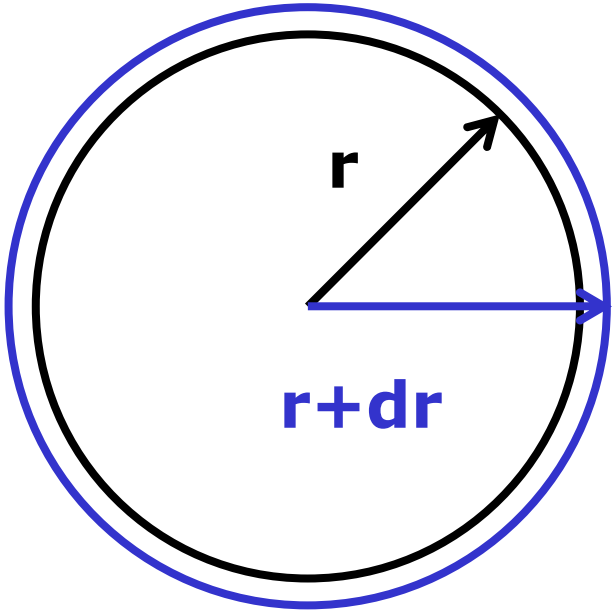

dv
r
Núcleo

Distribuição de Probabilidade para o Orbital 1s

Ψ^2_{1s}

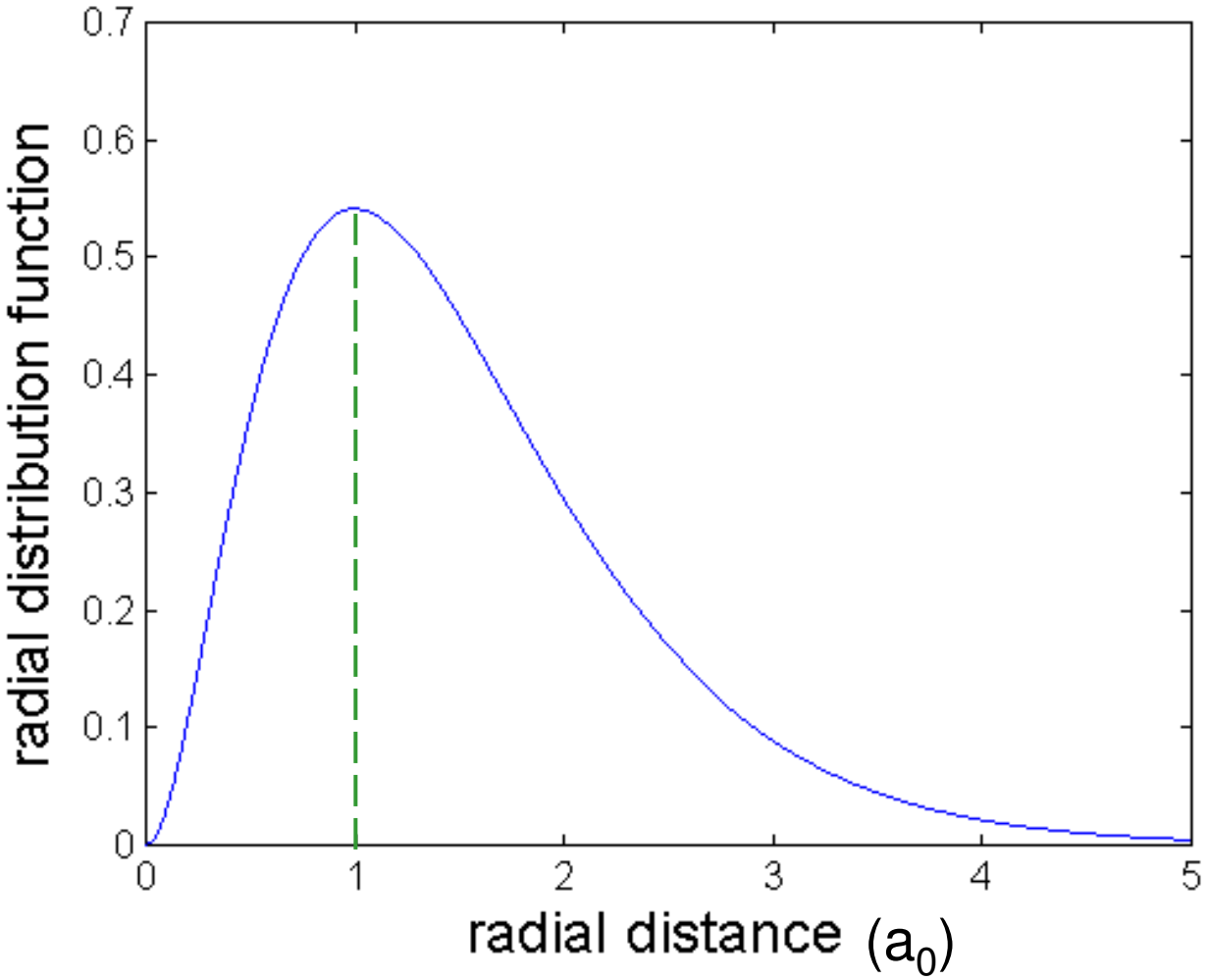


Função de Distribuição Radial (casca)



Função de Distribuição Radial

$4\pi r^2 \psi^2_{1s}$



Achtung!!!

Attenzione!!!

Caution!!!

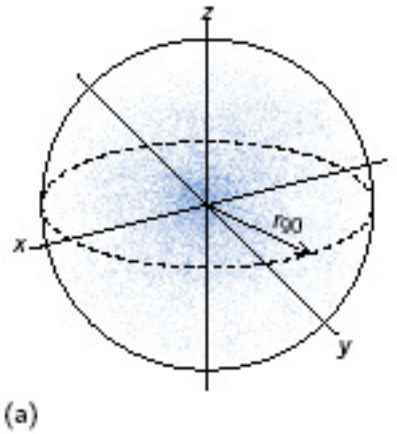
Densidade de Probabilidade

X

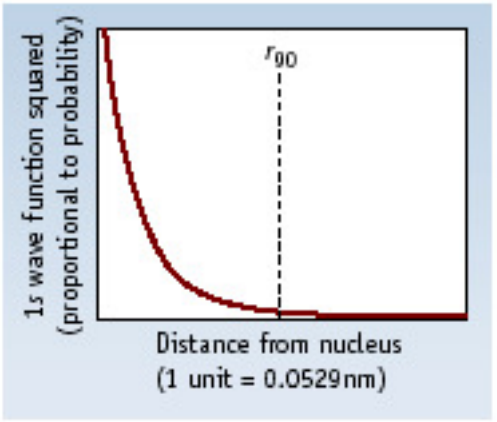
Densidade de Probabilidade Radial

(Função de Distribuição Radial)

Nuvem (dots)

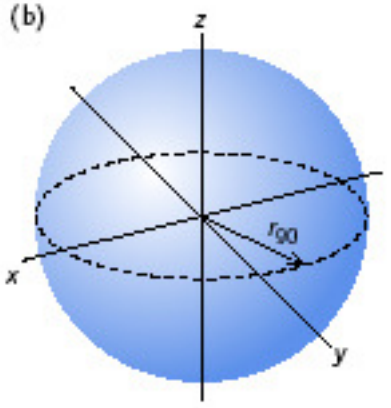


(a)



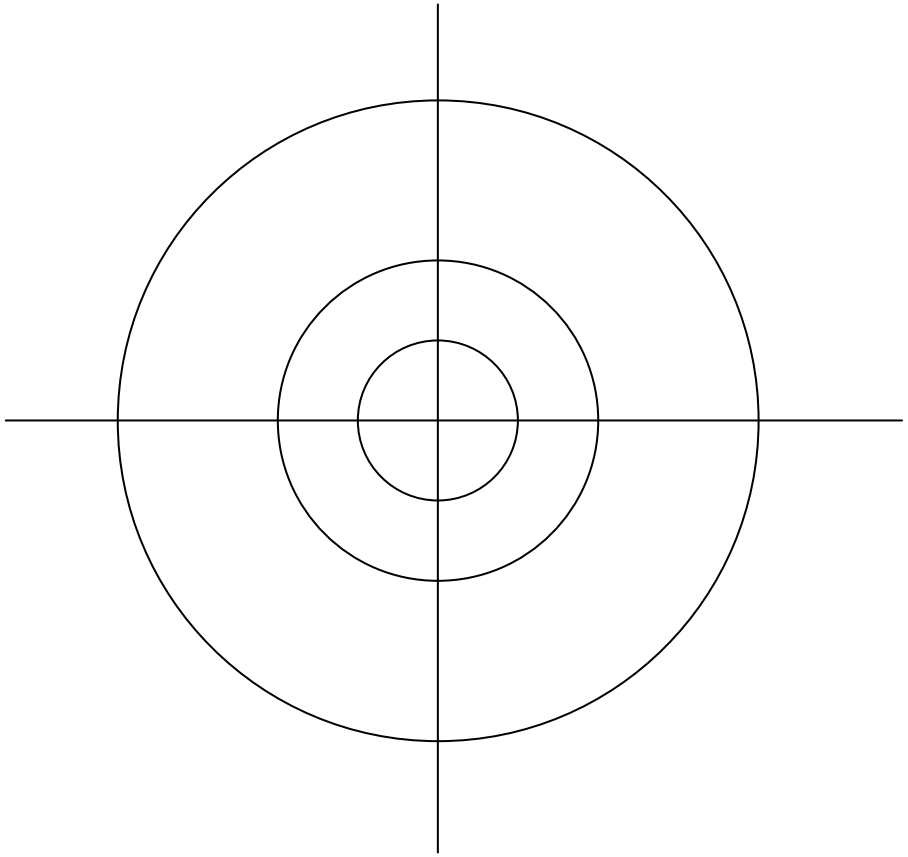
(b)

Superfície Limite

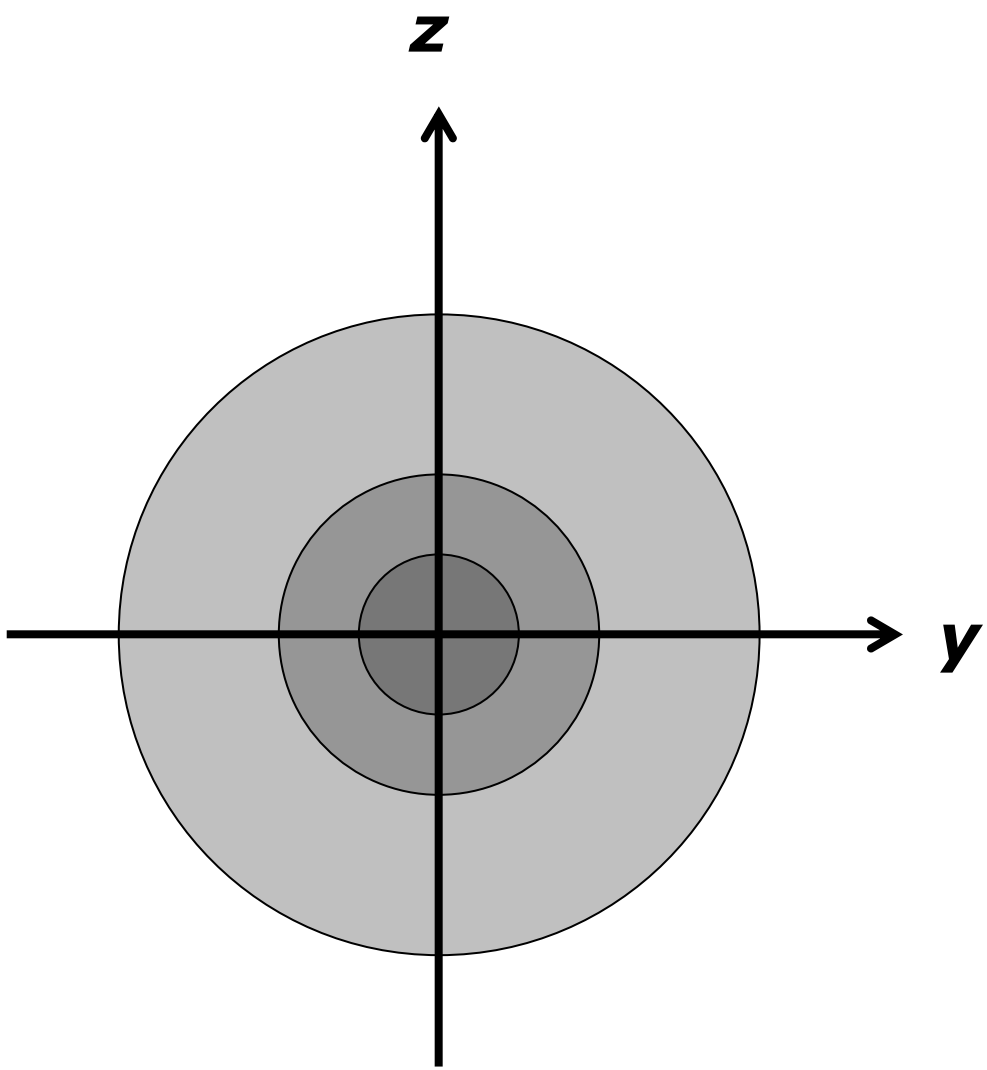


(c)

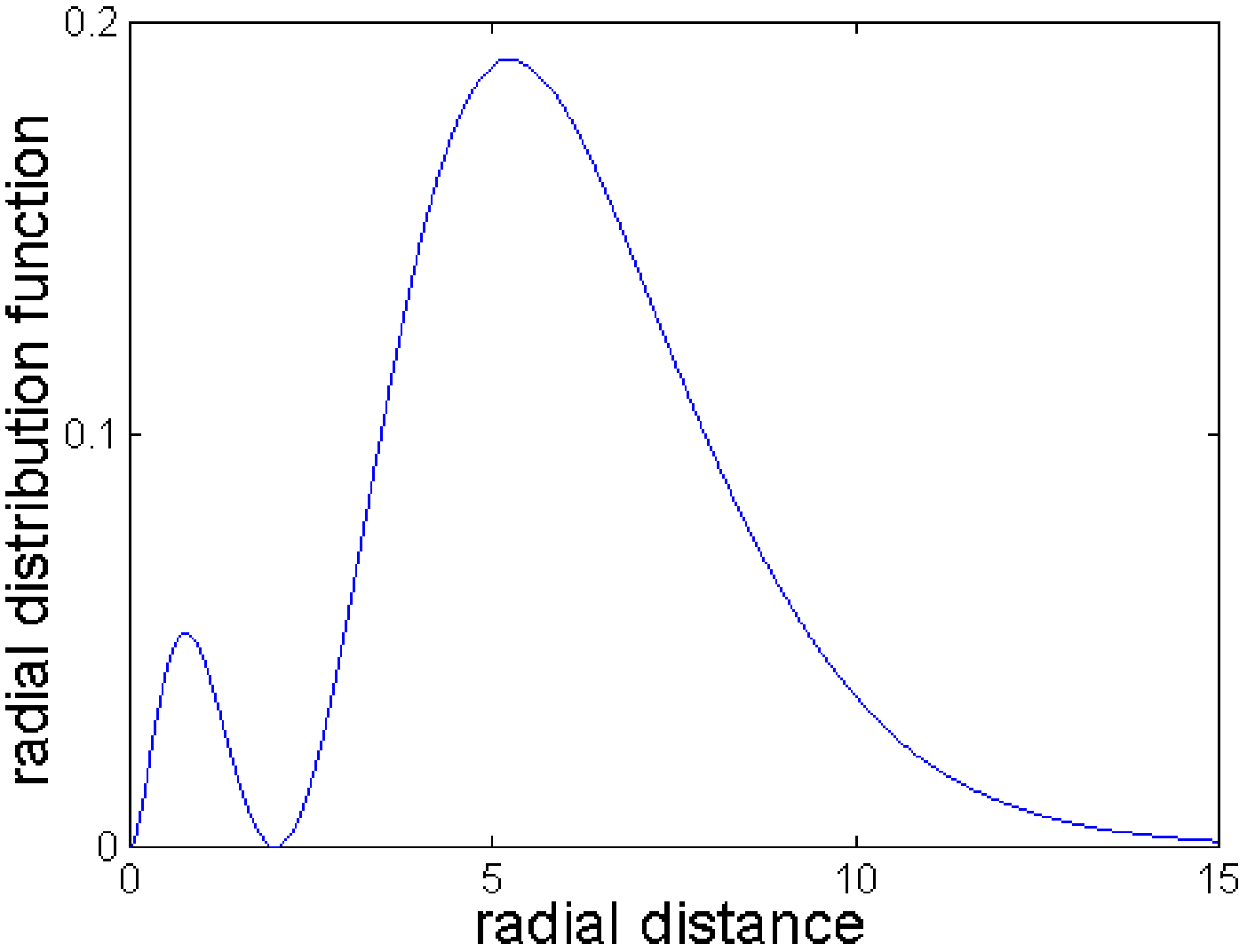
Diagramas de Contorno



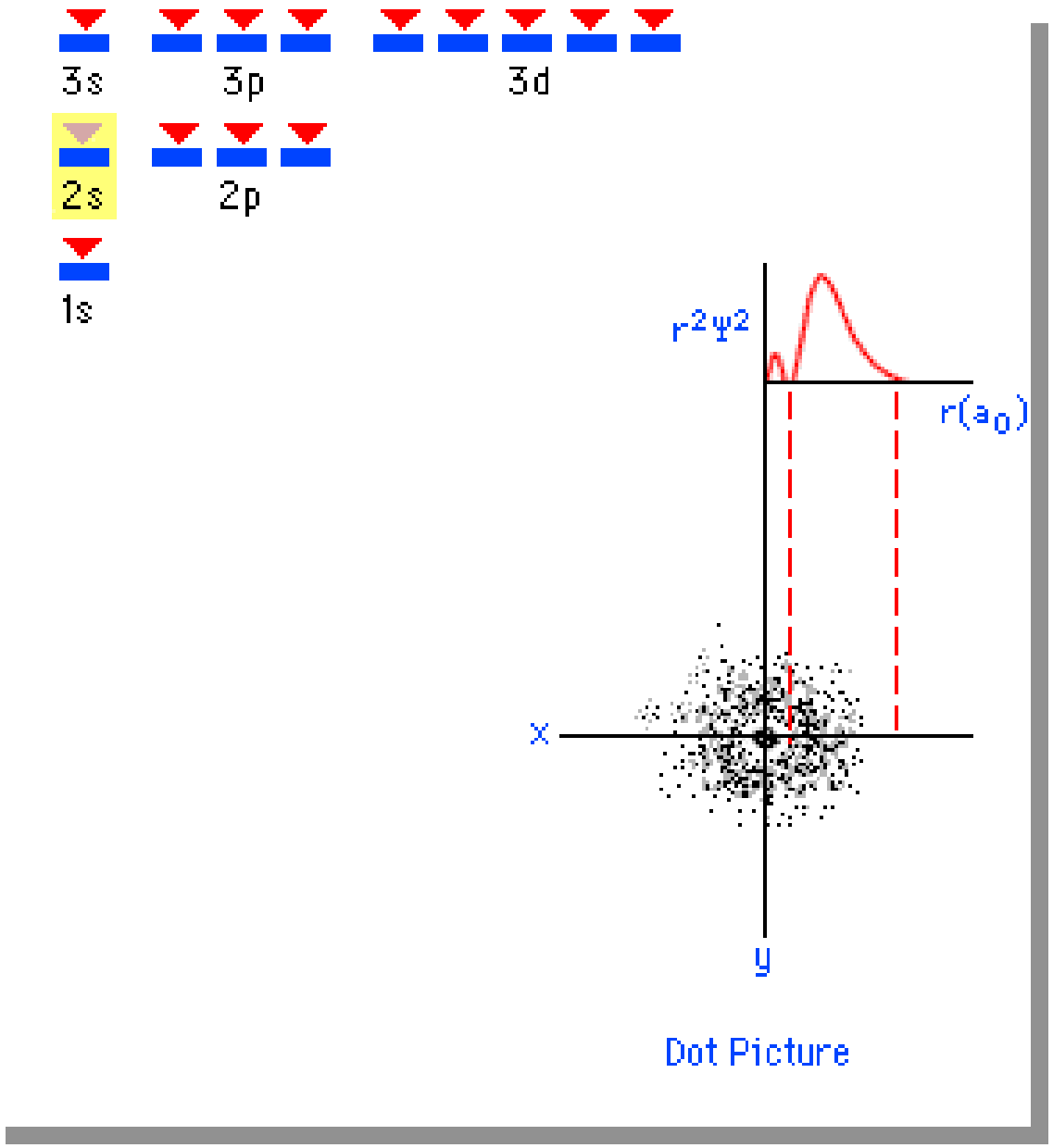
Diagramas de Contorno



Função de Distribuição Radial: Orbital 2s



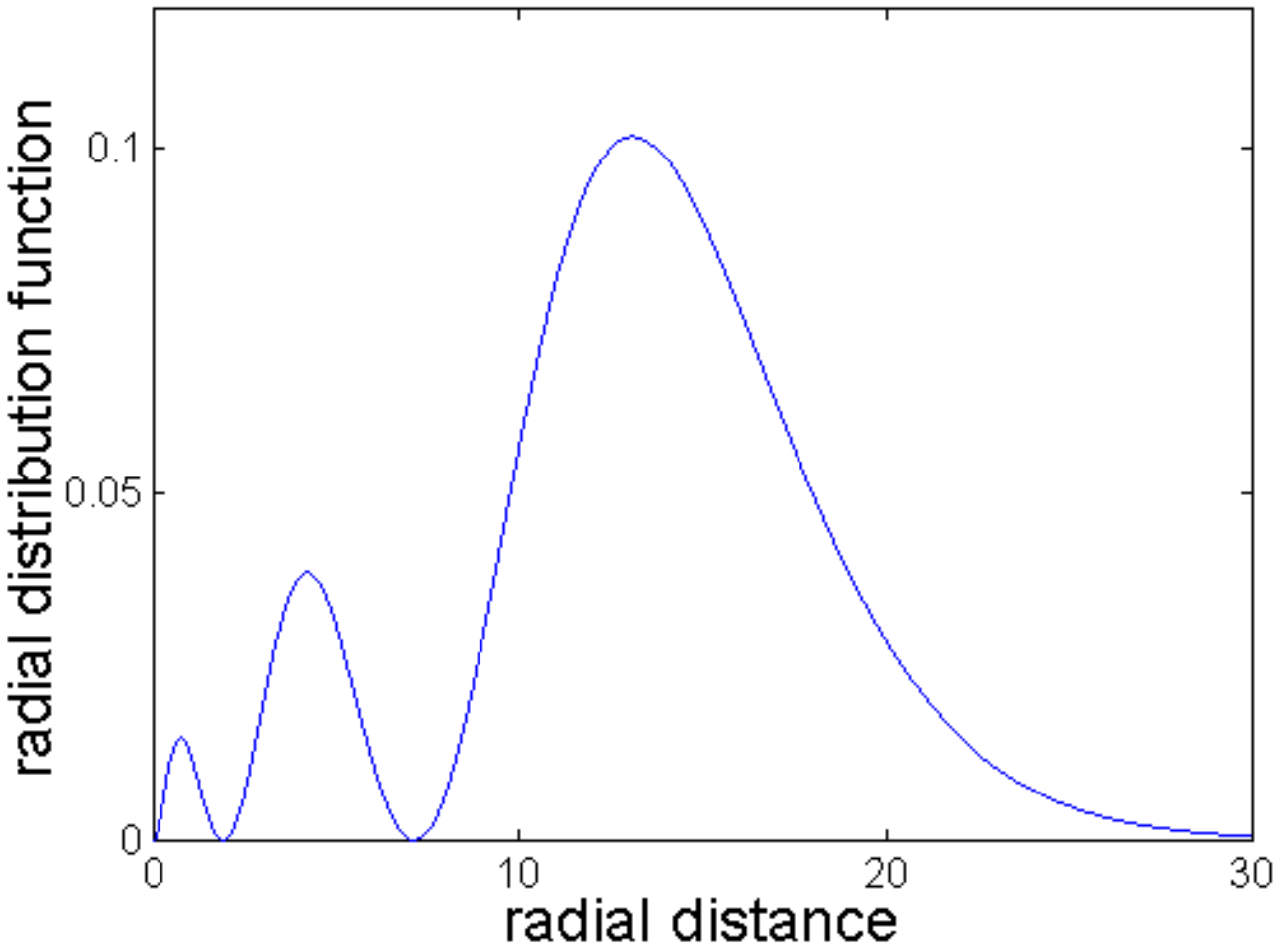
Orbital 2s

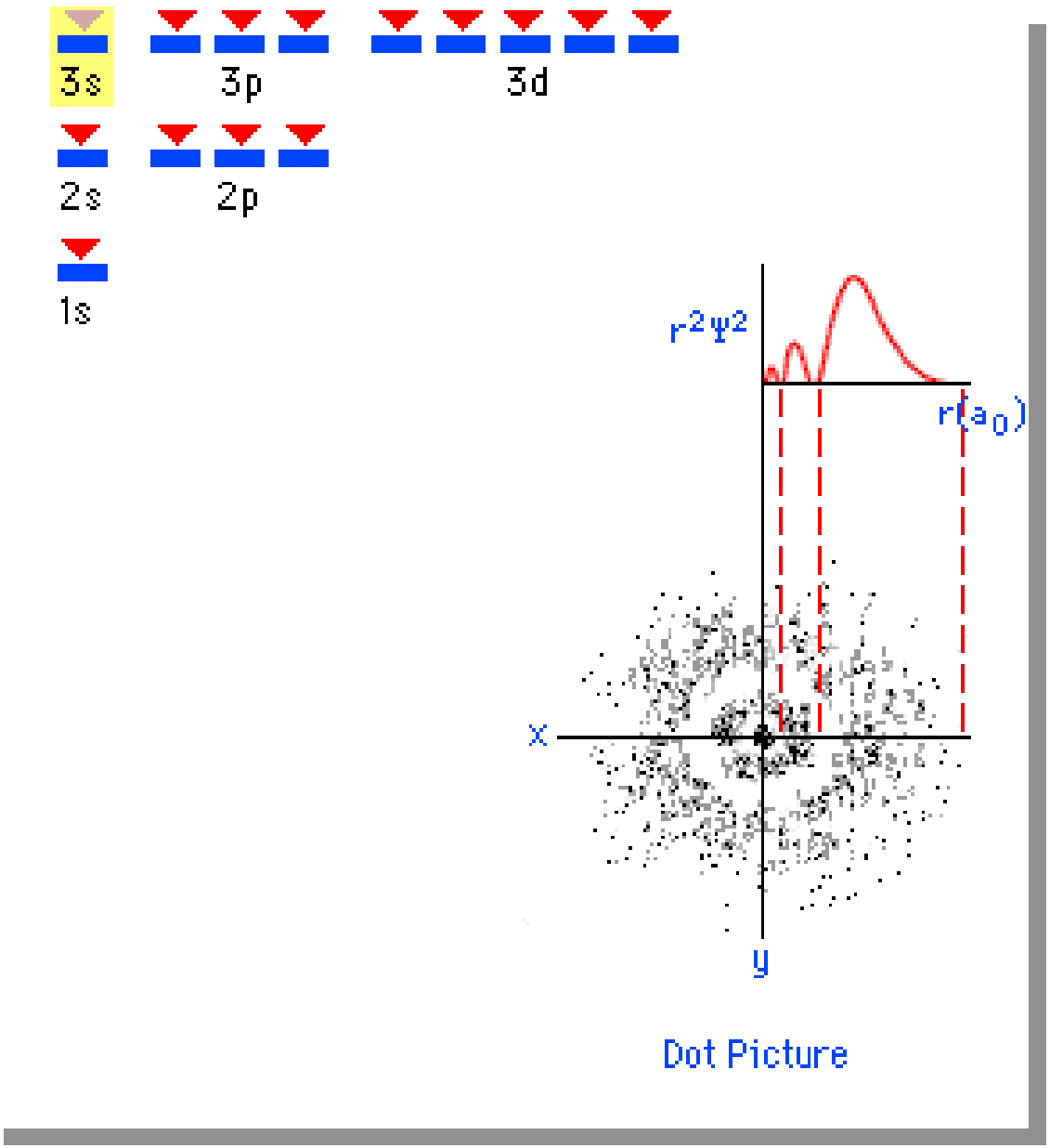


Distribuição Radial

Densidade Eletrônica

Função de Distribuição Radial: Orbital 3s





Orbital 3s

Distribuição Radial

Densidade Eletrônica

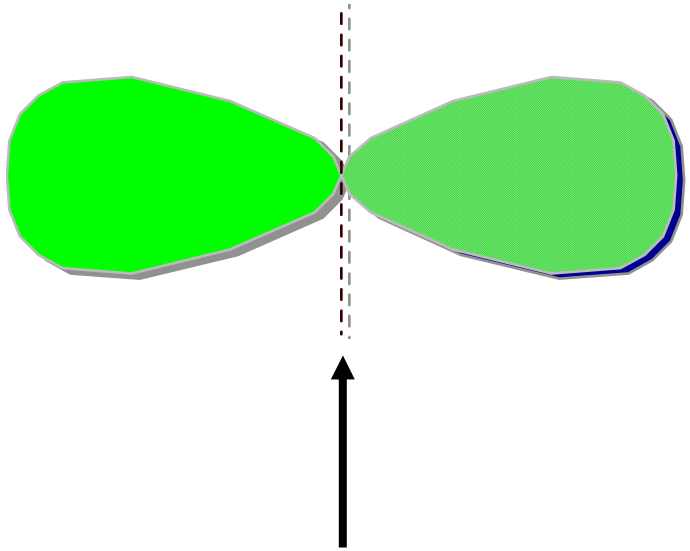
Orbitais p

Quando n=2

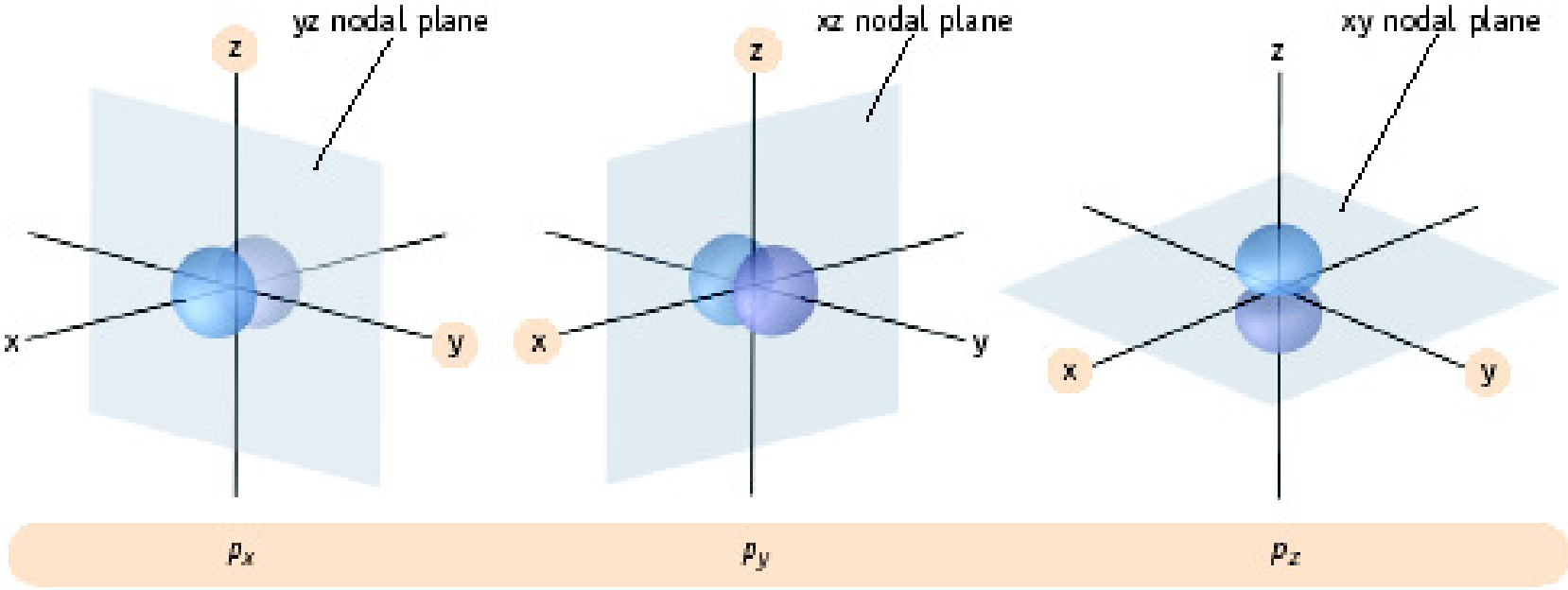
l=0 e 1

Para l= 1

m_l= -1, 0, 1

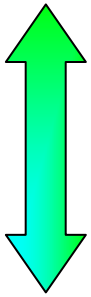


Plano Nodal
no Núcleo



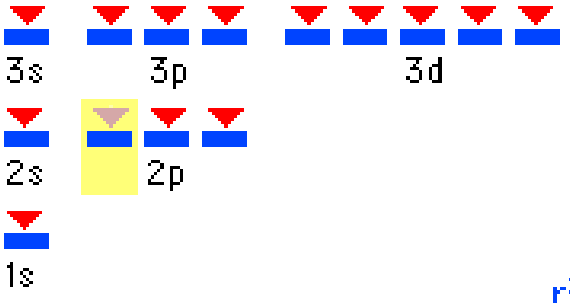
Orbitais p disposicionados a 90º

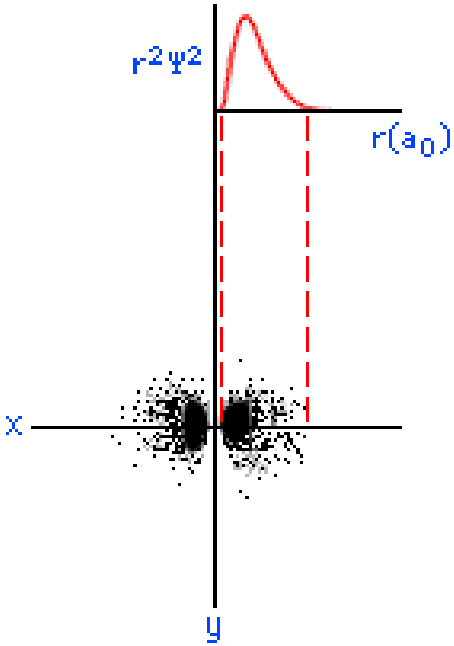
Orbitais Degenerados



Mesma Energia

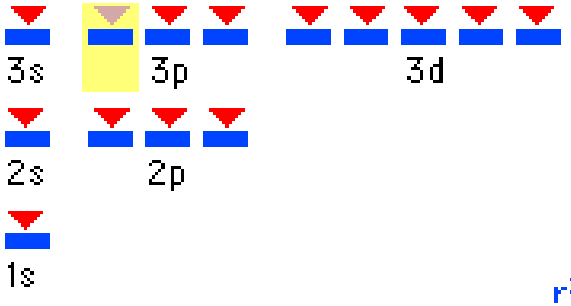
Orbital $2p_x$

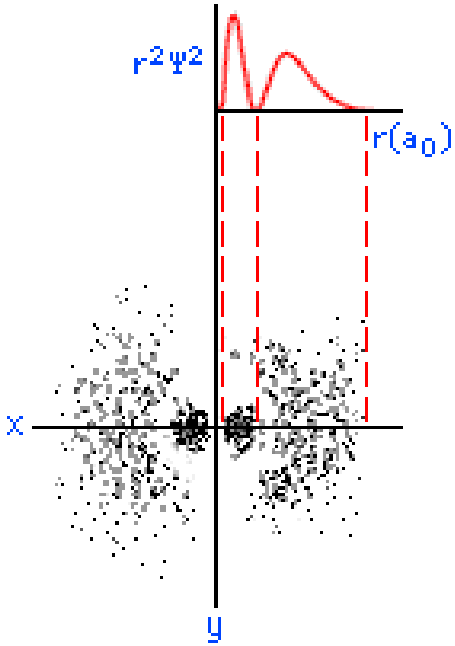




Dot Picture

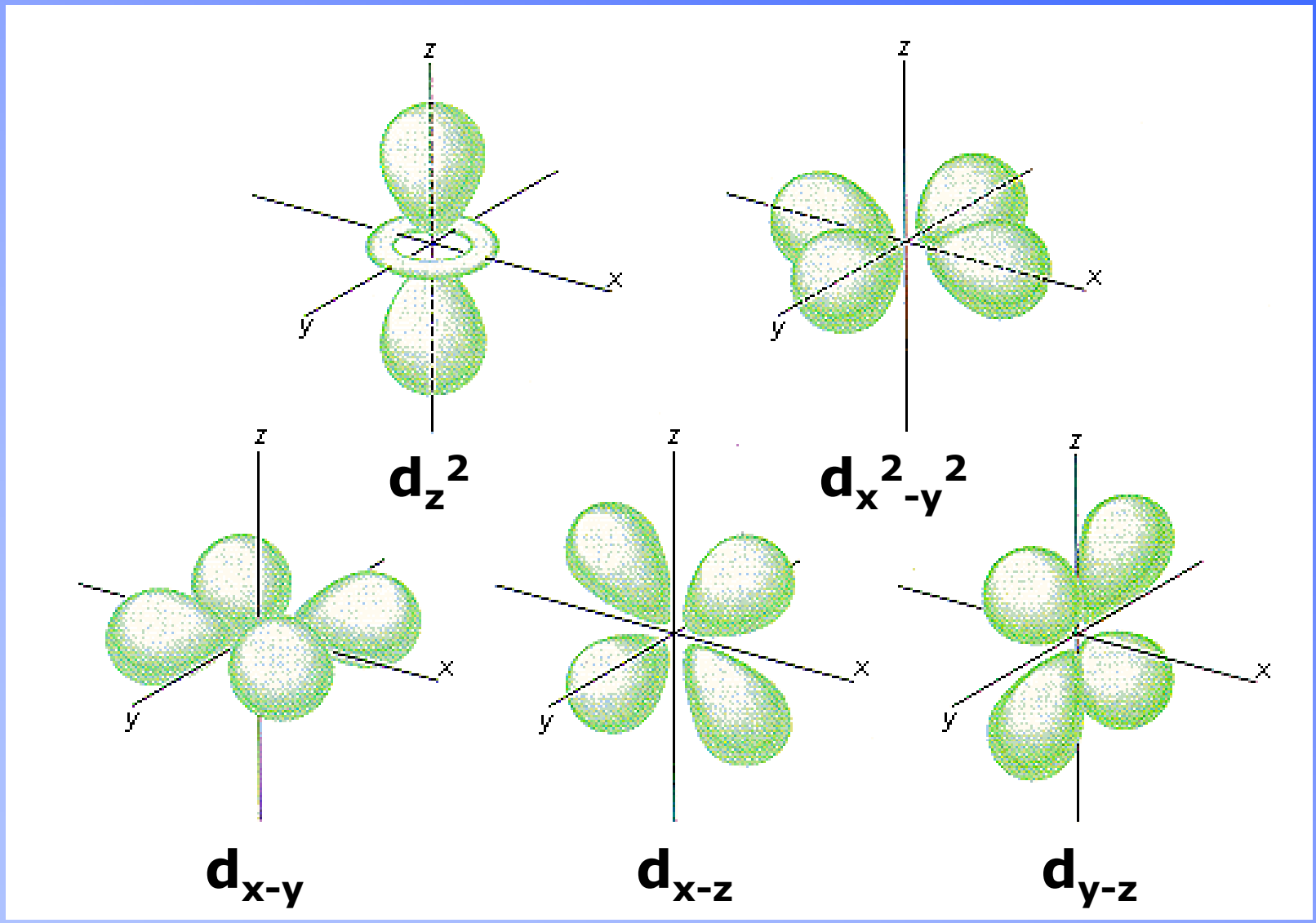
Orbital $3p_x$



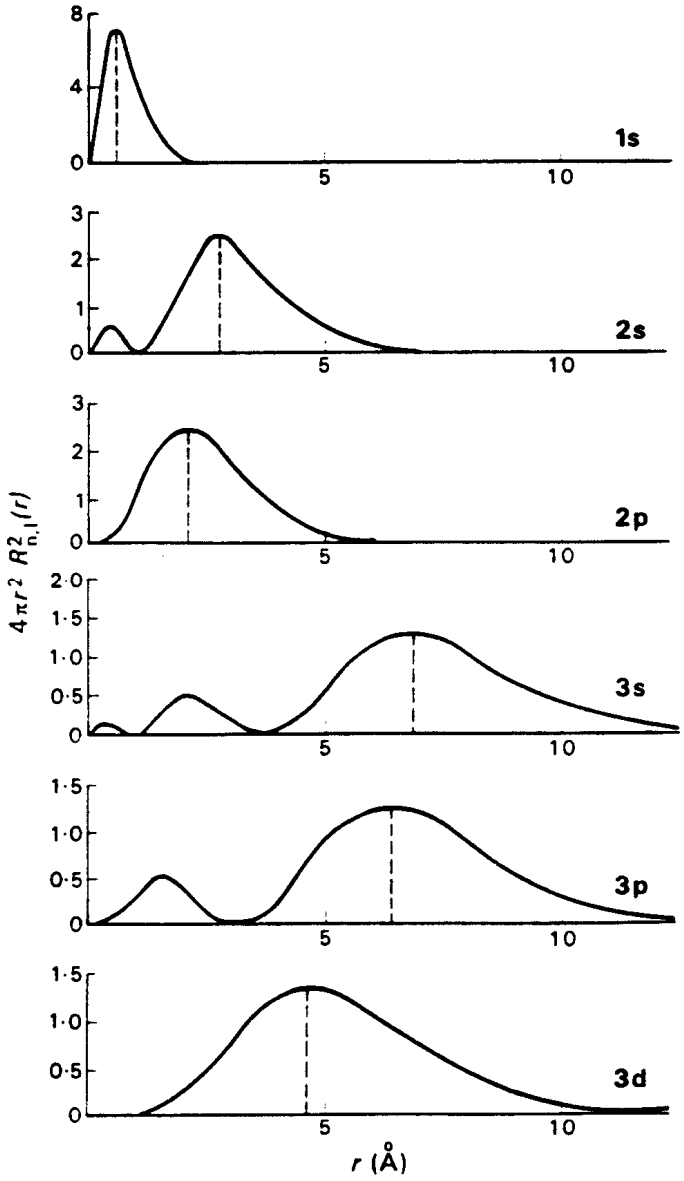


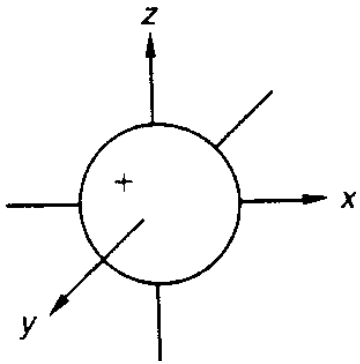
Dot Picture

Disposição Espacial dos Orbitais d

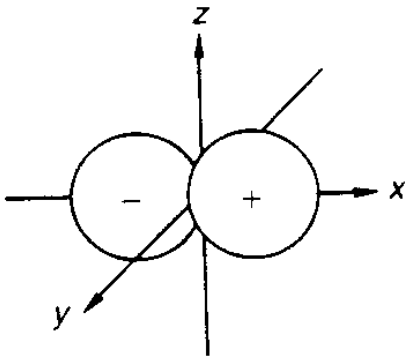


Função de Distribuição Radial

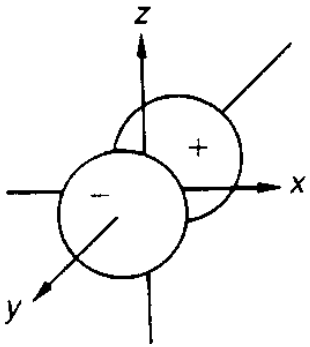




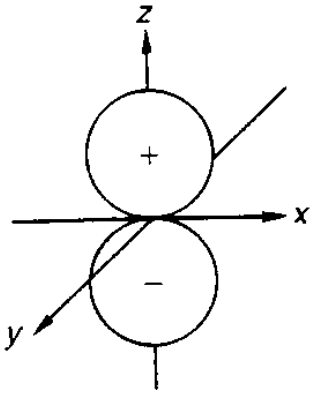
1*s*



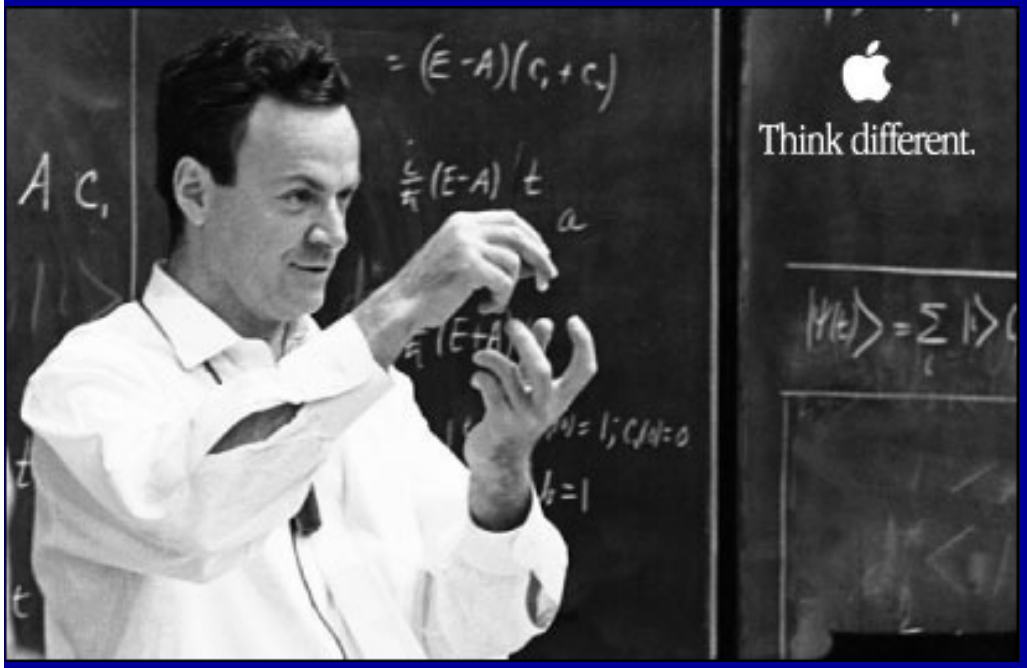
2p_x



2p_y



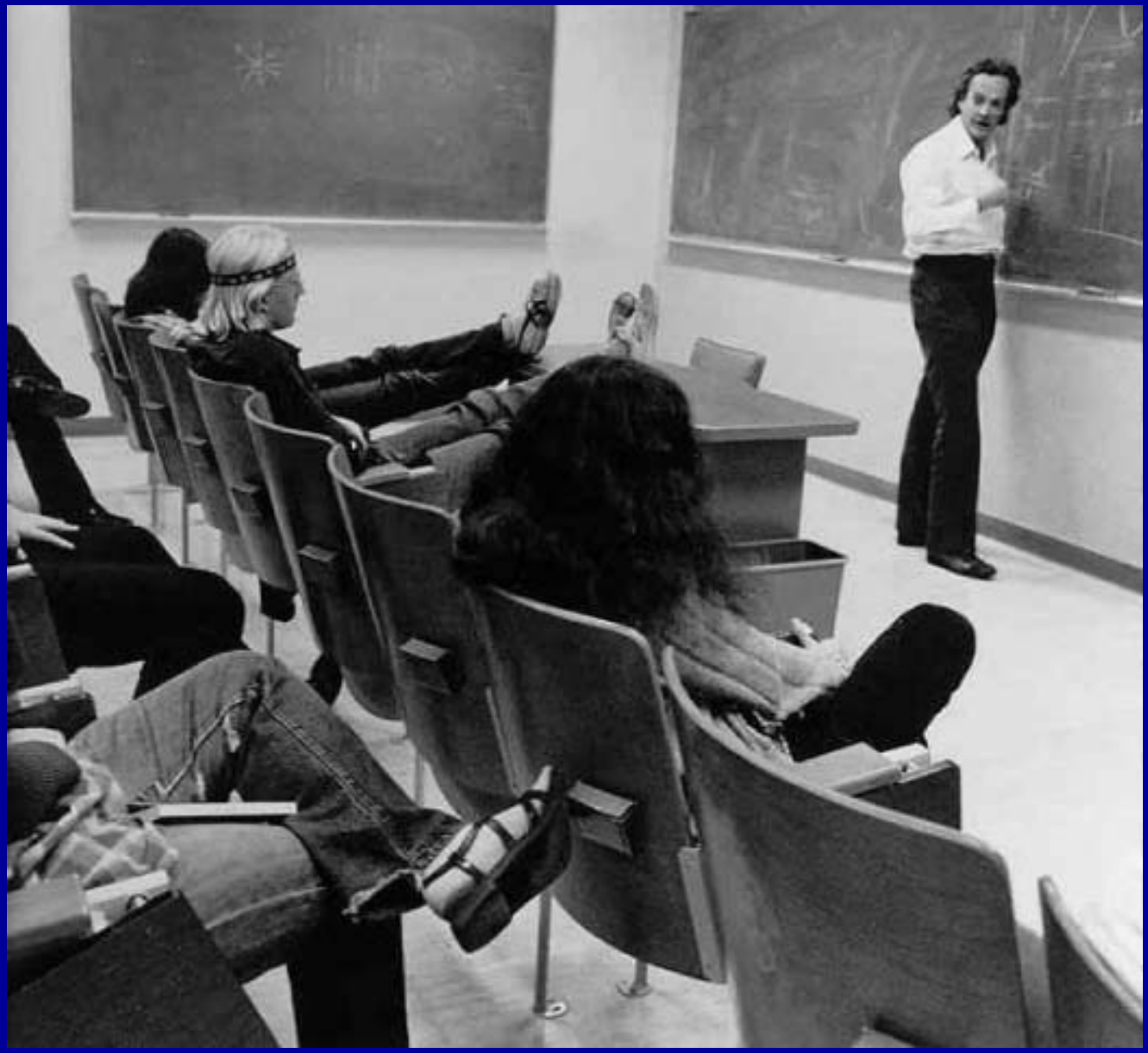
2p_z

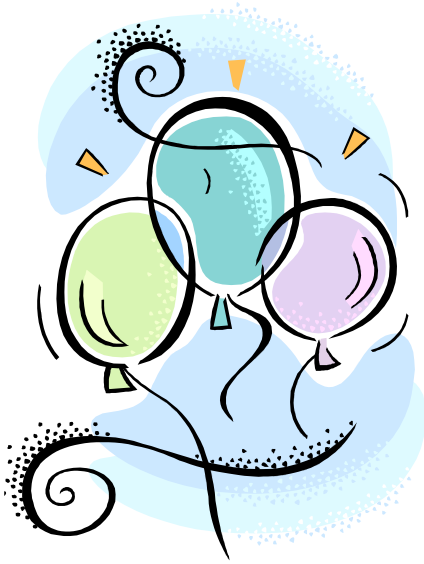


Richard Feynman:
Prêmio Nobel em Física
1965

Eletrodinâmica Quântica

"Acho que posso afirmar com segurança que ninguém entende a mecânica quântica"





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